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Title: LANL Institutional Computing 2020 Annual Status Report: Improved Time-Stepping Methods in Global to Regional Ocean Modeling

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Improved Time-Stepping Methods in Global to Regional Ocean Modeling

Annual Status Report, 2020
LANL Institutional Computing account w20_ocean_time_step
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Scientific and Programmatic Impact

Time stepping algorithms are an important part of ocean models, and strongly influence both the accuracy of solution and performance. There have been a number of projects investigating various improvements for ocean time-stepping schemes in the Model for Prediction Across Scales-Ocean (MPAS-Ocean), a component of the DOE Energy Exascale Earth System Model.

Ocean dynamics include fast surface gravity waves, which are two-dimensional, and slower internal waves, which are three-dimensional, so ocean models use a split time-stepping scheme that separates these barotropic and baroclinic modes for efficiency. MPAS-Ocean runs on variable-resolution horizontal meshes, and must scale to tens of thousands of cores and millions of horizontal gridcells. Ocean models require time stepping algorithms that are customized to these needs, and which are tuned for performance on various resolutions and architectures.

Here we summarize each project using LANL Institutional Computing resources, account w20_ocean_time_step.

Local Time Stepping
Giacomo Capodaglio, post-doc, Mark Petersen, advisor
One of the major challenges for the simulation of coastal processes is the presence of sharp horizontal gradients that require the use of grid cells with size of tens of meters to appropriately describe the physics. On the other hand, the phenomena occurring in the vicinity of the coast are very much tied to the ocean behavior at a global level. Multiresolution global ocean simulations are currently possible with MPAS-O, although the largest time-step that allows stability is constrained by the size of the smallest cell in the grid, according to the CFL condition. To overcome this issue, a local time stepping (LTS) scheme specifically designed for MPAS-O has been recently integrated in MPAS-O. We have made progress on implementational design choices as well as quantitative results and performance associated with the use of the LTS scheme.

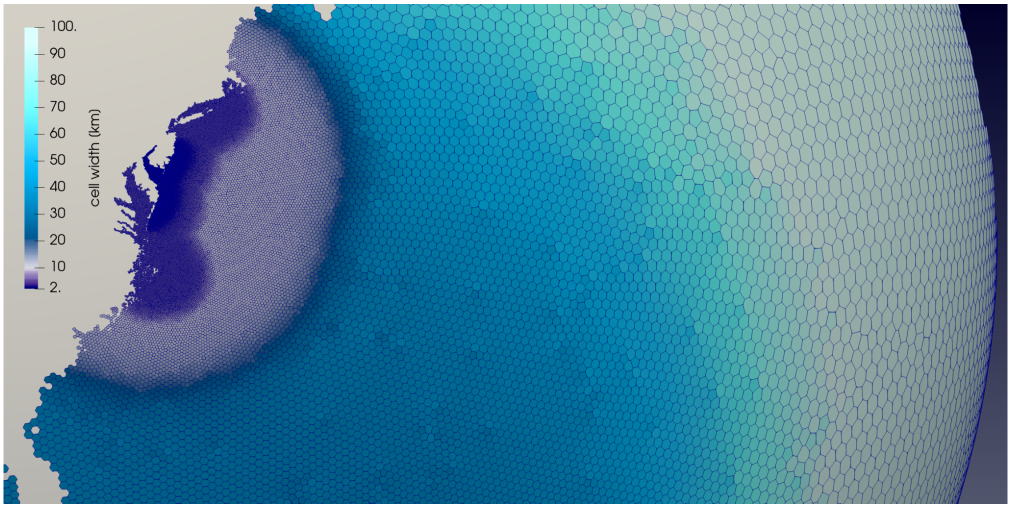

Figure 1. MPAS variable-resolution mesh on the east coast of the US, with 2 km resolution in Deleware Bay. Local time stepping is currently being tested with the shallow water equations. The next step is to test in global ocean simulations.

A Suite of Verification Exercises for Barotropic Solver of Ocean Models
Siddhartha Bishnu, graduate student (LANL, Fl. State), Mark Petersen
Abstract: The development of any numerical ocean model warrants a suite of verification exercises for testing its spatial and temporal discretization. We have developed a set of shallow water test cases designed for verifying the barotropic solver of unstructured ocean models. These include dispersive and non-dispersive geophysical waves and barotropic tides for testing the implementation of the linear pressure gradient terms as well as the linear but possibly variable-coefficient Coriolis and bathymetry terms. Standard test cases like the implementation of the heat equation, the viscous Burger's equation and manufactured solutions are also used for testing the non-linear advection terms, the linear variable-coefficient diffusion terms and complex bathymetry. Special care needs to be taken while implementing the non-periodic boundary conditions on unstructured meshes. We have created convergence plots of every test case in space and time at constant ratio of time step to grid spacing for a variety of time-stepping algorithms.

A modified TRiSK scheme to address instabilities found in MPAS-Ocean
Sara Calandrini, post-doc, Mark Petersen, Darren Engwirda
In MPAS-O the horizontal discretization used is the TRiSK scheme, a C-grid, finite-volume method applied to Spherical Centroidal Voronoi Tessellations (SCVTs) where the mass, tracers, pressure and kinetic energy are defined at centers of the convex polygons and the normal component of velocity is located at cell edges. This method has many desirable mimetic properties, in spite of possessing low order of accuracy and inconsistencies that may constitute a potential problem for high resolution 3D models. In this work, we investigate a modification for the TRiSK scheme that will make it first order accurate in the maximum norm. Simulations compare the modified versus the original scheme for accuracy and stability.

Exponential Integrators for the Solution of the Tracer Equations in MPAS-Ocean
Sara Calandrini, post-doc, Phil Jones, Mark Petersen
Exponential time differencing (ETD) methods, also known as exponential integrators, constitute a class of numerical methods for the time integration of stiff systems of differential equations. Exponential integrators have recently gained attention in the ocean modeling community due to their stability properties that allow time steps considerably larger than those dictated by the CFL condition. We now have results obtained when such a scheme is applied within a full ocean circulation model.

On the Spatial and Temporal Order of Convergence of Hyperbolic PDEs
Siddhartha Bishnu, graduate student (LANL, Fl. State), Mark Petersen
This project computes the leading order terms of the local truncation error of hyperbolic partial differential equations (PDEs) on a uniform mesh. When employing a stable numerical scheme, we make the following observations in the asymptotic regime, where the truncation error is dominated by the powers of the grid spacing and the time step rather than their coefficients: (a) the order of convergence of stable numerical solutions of hyperbolic PDEs at constant ratio of time step to grid spacing is governed by the minimum of the orders of the spatial and temporal discretizations, and (b) convergence cannot be attained under only spatial or temporal refinement. We test our theory against numerical methods employing Method of Lines for any hyperbolic PDE, be it linear or non-linear, and employing finite difference, finite volume, or finite element discretization in space, and advanced in time with forward Euler, predictor-corrector, and multistep methods.

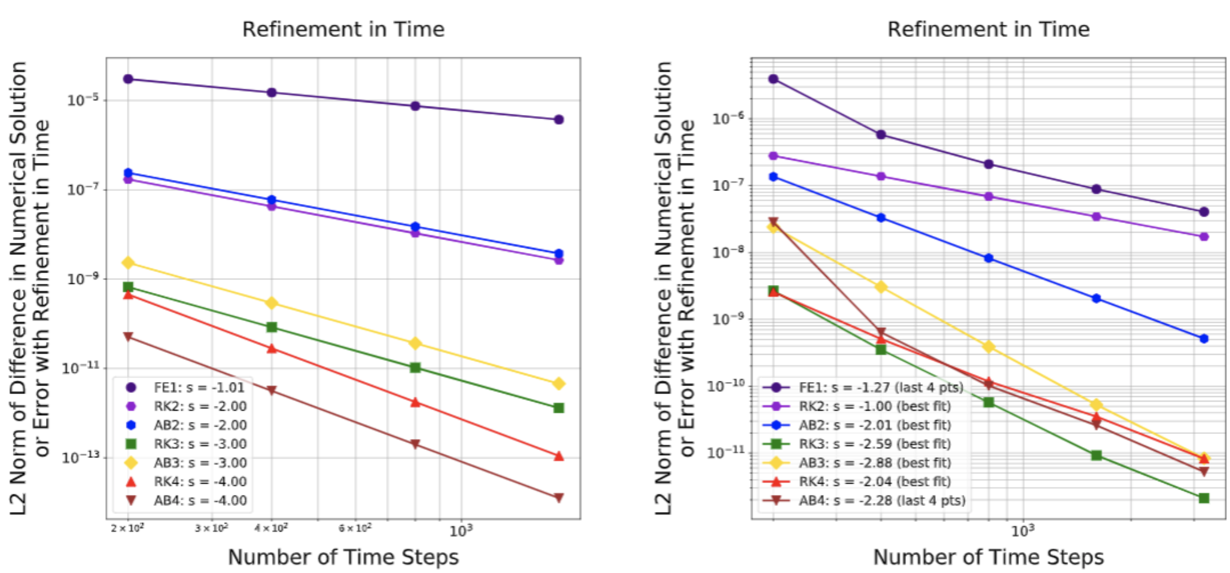

Figure 2. Convergence plots of the non-linear advection equation using first-order upwind (left) and fourth-order accurate piecewise parabolic reconstruction (right). From Bishnu et al. [1].

Publication List

Publications

1. On the Spatial and Temporal Order of Convergence of PDEs Part 1: Hyperbolic PDEs, Siddhartha Bishnu, Mark Petersen, Bryan Quaife. Submitted to Journal of Computational Physics
2. Local time stepping for the shallow water equations in MPAS-Ocean, Giacomo Capodaglio, Mark Petersen, in preparation for Ocean Modeling
3. A Suite of Verification Exercises for the Barotropic Solver of Ocean Models. Siddhartha Bishnu, Mark Petersen, Bryan Quaife, in preparation for Journal of Advances in Modeling Earth Systems

Presentations

1. A modified TRiSK scheme to address instabilities found in MPAS-Ocean, ESMD Meeting, Sara Calandrini, Mark Petersen, Darren Engwirda, October 26 2020
2. Local Time Stepping Schemes for Global to Coastal Simulations in MPAS-Ocean, Giacomo Capodaglio, Mark Petersen SIAM CSE21 Date: Wednesday, March 3 2021.
3. Visualization of Geophysical Waves and Tides in Ocean Models, Siddhartha Bishnu, Mark Petersen, FSU Fellows Society Fall 2020 Virtual Research Sharing
4. Exponential Integrators for the Solution of the Tracer Equations in MPAS-Ocean, SIAM CSE, Sara Calandrini, Phil Jones, Mark Petersen, March 3rd, 2021
5. Local Time Stepping Schemes for Global to Coastal Simulations in MPAS-Ocean. Giacomo Capodaglio, Mark Petersen, Poster at E3SM PI Meeting 2020, Oct 27, 2020.
6. Time-Stepping Methods for PDEs and Ocean Models, Siddhartha Bishnu, COSIM Webinar Series (Virtual) at LANL, March 2021
7. A Suite of Verification Exercises for Barotropic Solver of Ocean Models. Siddhartha Bishnu, Mark Petersen, Bryan Quaife, SIAM Conference on Computational Science and Engineering 2021 i.e. CSE21 (Virtual)
8. On the Spatial and Temporal Order of Convergence of Hyperbolic PDEs. Siddhartha Bishnu, Mark Petersen, Bryan Quaife, Computational Xposition 2021, Department of Scientific Computing, Florida State University (Virtual)

Financial Impact

The w20_ocean_time_step account supports the computational work of the following people and associated projects. All funding is under Office of Science, Office of Biological and Environmental Research (BER)

1. Mark Petersen: supported as part of the Energy Exascale Earth System Model (E3SM) project, and Integrated Coastal Modeling (ICOM)
2. Siddhartha Bishu: supported by the SciDAC projects LEAP (Launching an Exascale ACME Prototype) and CANGA (Coupling Approaches for Next Generation Architectures)
3. Giacomo Capodaglio: supported by Integrated Coastal Modeling ICOM
4. Sara Calandrini: supported by SciDAC project LEAP (Launching an Exascale ACME Prototype)
5. Nairita Pal: supported by Integrated Coastal Modeling ICOM